Vita

Candidate's name:

Universities Attended:

Hamidreza Parsimehr

University of Qom (2014) Bachelor of Science in applied chemistry

Iran Polymer&Petrochemical Inst. (2017) Master of science in polymer chemistry

University of New Brunswick (2023) Masters of Science

Publications:

Parsimehr, Hamidreza, et al. "Waste-to-Wealth: Wheat-Based Porous Electrodes for Electrochemical Energy Storage Devices." ECS Advances 2.2 (2023): 020503.

Moharramnejad, Mojtaba, et al. "Cobalt-based electroactive compounds: synthesis and their electrochemical and pseudocapacitance performance." Journal of Materials Science: Materials in Electronics 34.6 (2023): 499.

Moharramnejad, Mojtaba, et al. "Zinc-based metal-organic frameworks: Synthesis and recent progress in biomedical application." Journal of Inorganic and Organometallic Polymers and Materials 32.9 (2022): 3339-3354.

Parsimehr, Hamidreza, et al. "Stimuli-Responsive Electrochemical Energy Storage Devices." The Chemical Record 22.9 (2022): e202200075.

Rastegar, Niloofar, et al. "Sound-absorbing porous materials: a review on polyurethane-based foams." Iranian Polymer Journal (2022): 1-23.

Parsimehr, Hamidreza, et al. "Electrochemical energy storage electrodes from rice biochar." Biomass conversion and biorefinery (2022): 1-17.

Carbonized Metal-Organic Frameworks as Bifunctional Electrocatalysts for **Oxygen reduction/Evolution Reactions**

UNIVERSITY OF NEW BRUNSWICK

THESIS DEFENCE AND EXAMINATION

in Partial Fulfillment

of the Requirement for the Degree of Master of Science

by

Hamidreza Parsimehr

in the Department of Chemistry

U.N.B., Fredericton, N.B.

Tuesday, October 24th, 2023 2:30 p.m.

Tilley Hall, Room 5

Examining Committee Dr. Anna Ignaszak Dr. Stijn de Baerdemacker Internal Examiner Dr. Zahra Khatami Dr. Gilles Villemure

Supervisor Int-Ext Examiner Chair of Oral Examination

Abstract

Electrochemical energy devices as a benign highperformance solution for energy issues have been swiftly developed in recent decades. Batteries have been known as an appropriate method for electrochemical energy storage. Also, fuel cells have been considered an effective method of producing electrochemical energy. Both metal-air batteries (MABs) and fuel cells (FCs) use a positive electrode (cathode) that has a similar chemical composition to facilitate oxygen reduction reactions (ORR) during their operation. The second important reaction involving oxygen species is the oxygen evolution reaction (OER) which is used in water electrolyzers to generate oxygen. An electrocatalyst incorporated in the electrodes in the above-listed energy systems is key to the efficient ORR and OER processes. Such electrocatalyst plays a critical role in overall performance, stability, and long cycle lifetime.

This research project is focused on developing a new class of ORR and OER electrocatalysts that can replace very

expensive commercial electrocatalysts such as platinum and ruthenium. The main objective is to evaluate the electrochemical performance of heteroatom-doped carbons such as Cu-N-doped carbon made by pyrolysis of metal-organic frameworks (MOFs), and Co-N-doped carbon, Fe-N-doped carbon, and Co/Fe-Ndoped carbon catalysts derived from zeolitic imidazole frameworks (ZIFs). We used a solvent-free synthesis of ZIFs to prepare Co-N-, Fe-N-, and Co/Fe-N-doped carbons. The electrochemical characteristic showed that the pyrolyzed Cobalt ZIF and the pyrolyzed Cobalt-Iron ZIF have the best ORR and OER activity. Further work is needed to prove that Co-N-C and Fe-N-C catalytic centers are present in these materials, and further optimization of the pyrolysis conditions are required to avoid precipitation of Co and Fe metallic particles.

If successfully developed, these heteroatom-doped carbonaceous materials hold the promise to replace expensive Pt/Ru-based electrocatalysts that will accelerate the massive production of fuel cells, MABs, and water electrolyzers.



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